

# Local field factors in a polarized two-dimensional electron gas

Juana Moreno and D. C. Marinescu

*Department of Physics, Clemson University, Clemson, SC 29634*

(Dated: February 1, 2008)

We derive approximate expressions for the static local field factors of a spin polarized two-dimensional electron gas which smoothly interpolate between their small- and large-wavevector asymptotic limits. For the unpolarized electron gas, the proposed analytical expressions reproduce recent diffusion Monte Carlo data. We find that the degree of spin polarization produces important modifications to the local factors of the minority spins, while the local field functions of the majority spins are less affected.

PACS numbers: 71.10.-w, 72.25.-b, 71.45.Gm

## I. INTRODUCTION

In most of the many body theories of electronic systems, the spin polarization in a magnetic field has been considered as a small parameter. This picture is certainly true when the Zeeman splitting is much smaller than other relevant energies in the problem. However, recently, attention has been focused on materials where the Zeeman splitting dominates the energy spectrum, such as the diluted magnetic semiconductors. The large Zeeman splitting is due to the strong exchange interactions between the itinerant carriers and the magnetic ions that generate a value of the effective gyromagnetic factor,  $\gamma^*$ , up to hundreds of times its band value. As a consequence, even in weak magnetic fields these systems can be fully polarized.<sup>1</sup> Due to their easy polarizability these materials are promising candidates to accomplish spin dependent conduction in solid state devices;<sup>2</sup> hence the interest in developing an appropriate microscopic model for them.

A realistic picture of the spin polarized electron gas hinges on finding an appropriate description of the many-body interaction, which has to incorporate the explicit spin dependence of the short range Coulomb repulsion. In this paper, we examine these short range effects in a two dimensional polarized electron gas. The self-consistent treatment of the exchange and correlation effects has proven to be very important in understanding the physics of normal metals,<sup>3</sup> but to our knowledge it has not been fully analyzed in spin-polarized systems. In addition, the relevance of the exchange and correlation effects increases as the dimensionality of the electron gas is lowered.

We model the exchange (x) and correlation (c) hole around each electron by using spin dependent local field correction functions,  $G_{\sigma}^{x,c}(\mathbf{q}, \omega)$ .<sup>4</sup> They describe the difference between the true particle density and its mean field (RPA) counterpart. The spin dependence of these factors is a consequence of the fact that the microscopic interaction is different for up and down spin electrons. The microscopic origin of the local field corrections was elucidated by Kukkonen and Overhauser.<sup>5</sup> In a direct generalization of this approach, the effective potential  $\tilde{\mathcal{V}}_{\sigma}$

experienced by an electron with spin  $\sigma$  in the presence of external electric  $[\phi(\mathbf{q}, \omega)]$  and magnetic fields  $[\vec{B}(\mathbf{q}, \omega)]$  can be written as:<sup>4,6</sup>

$$\tilde{\mathcal{V}}_{\sigma}(\mathbf{q}, \omega) = -e\phi(\mathbf{q}, \omega) + \gamma^* \vec{\sigma} \cdot \vec{B}(\mathbf{q}, \omega) +$$

$$v(\mathbf{q}) \left\{ [1 - \tilde{G}_{\sigma}^{+}(\mathbf{q}, \omega)] \Delta n(\mathbf{q}, \omega) - \vec{\sigma} \cdot \Delta \vec{m}(\mathbf{q}, \omega) \tilde{G}_{\sigma}^{-}(\mathbf{q}, \omega) \right\} \quad (1)$$

where  $\Delta n = \Delta n_{\uparrow} + \Delta n_{\downarrow}$  and  $\Delta \vec{m}$  are, respectively, the density and the magnetization fluctuation induced by the external fields,  $\vec{\sigma}$  are the Pauli spin matrices and  $v(\mathbf{q})$  is the bare Coulomb interaction,  $2\pi e^2/\mathbf{q}$ . The local field factor  $\tilde{G}_{\sigma}^{+}(\mathbf{q}, \omega)$  is the sum of parallel- and antiparallel-spin effects, while  $\tilde{G}_{\sigma}^{-}(\mathbf{q}, \omega)$  is the difference of parallel- and antiparallel-spin effects:  $\tilde{G}_{\sigma}^{\pm}(\mathbf{q}, \omega) = \tilde{G}_{\sigma}^x \pm \tilde{G}_{\sigma\sigma}^c$ .<sup>7</sup>

In a linear approximation, the density fluctuations are proportional to the effective potentials:  $\Delta n_{\uparrow} = \Pi_{\uparrow\uparrow} \tilde{\mathcal{V}}_{\uparrow}$  ( $\Delta n_{\downarrow} = \Pi_{\downarrow\downarrow} \tilde{\mathcal{V}}_{\downarrow}$ ),<sup>4,8</sup> where the proportionality coefficients are the polarization functions of the fully interacting electron system. Since the interacting polarization function is generally unknown, an additional local field factor ( $G_{\sigma}^n$ ) is needed to relate the interacting polarization function,  $\Pi_{\sigma\sigma}$ , with the non-interacting one,  $\Pi_{\sigma\sigma}^0$ , as in<sup>9</sup>

$$\Pi_{\sigma\sigma}(\mathbf{q}, \omega) = \frac{\Pi_{\sigma\sigma}^0(\mathbf{q}, \omega)}{1 + 2v(\mathbf{q})G_{\sigma}^n(\mathbf{q}, \omega)\Pi_{\sigma\sigma}^0(\mathbf{q}, \omega)} \quad (2)$$

This parameterization of the modified polarization function leads to a renormalized expression of the local fields that determine the response functions, such that the complete local field functions are given as:  $G_{\sigma}^{\pm} = \tilde{G}_{\sigma}^{\pm} + G_{\sigma}^n$ .<sup>9</sup>

Quantitative calculations of many physical properties require the precise knowledge of the local field correction functions. The determination of the frequency and wave vector dependence of the local field corrections is a very difficult problem which remains unsolved even in the case of the unpolarized electron system. Fortunately, the asymptotic values of the local field factors can be obtained exactly in some limiting cases.<sup>8,10,11</sup> Numerical estimates of the response functions of the two and three

dimensional unpolarized electron gas have shown that local field factors smoothly interpolate between the asymptotic small and large wave-vector behavior.<sup>12</sup> This feature is expected to exist also in the case of a spin polarized system, and, consequently, we use the asymptotic limits of the static local factors for large and small wavevector as a starting point in deriving their approximate expressions across the whole spectrum of momentum.

The fundamental parameters of the problem are the coupling strength,  $r_s = a_B^* / \sqrt{\pi(n_\uparrow + n_\downarrow)} = a_B^* / \sqrt{\pi n}$ ,<sup>13</sup> and the spin polarization,  $\zeta = (n_\uparrow - n_\downarrow) / n$ . Since the many body interaction is independent of the source of the polarization we expect our results to maintain their validity also in the case of an itinerant ferromagnet with a self-induced magnetic field, or when the polarization is achieved by other means, such as shining circularly polarized light on the sample.

In section II, we study the large and the small wavevector limits of the local field functions and their dependence with the electronic density and polarization. In section III, we give a simple parameterization of the local field factors which satisfy the asymptotic limits and reproduces the most recent numerical results for the unpolarized electron gas.<sup>12</sup> Section IV presents our conclusions.

## II. LIMITING BEHAVIOR OF THE LOCAL FIELD FACTORS

Our first approximation is to neglect the frequency dependence of the local field corrections. Although the local field functions represent a dynamical effect,<sup>9,14</sup> they vary slowly on the scale of the Fermi frequency,<sup>15,16</sup> and it is acceptable to neglect their frequency dependence if we are mainly interested in response functions.

### A. Small wavevector

At zero frequency and small wavevector, sum rules are used to connect the static limits of various response functions to certain thermodynamic coefficients, which can be expressed as derivatives of the ground state energy of the electron gas.<sup>10</sup> Subsequently, the renormalized local field functions, which are directly connected with these response functions, are written down as derivatives of the exchange and correlation energy of the interacting electron gas ( $E^{xc}$ ):

$$G_\sigma^+(\mathbf{q} \rightarrow 0) = \frac{\tilde{q} r_s^2}{8\sqrt{2}} \left( \frac{\partial \epsilon^{xc}}{\partial r_s} - r_s \frac{\partial^2 \epsilon^{xc}}{\partial r_s^2} + 2 \text{sign}(\sigma) \frac{\partial^2 \epsilon^{xc}}{\partial r_s \partial \zeta} \right), \quad (3)$$

$$G_\sigma^-(\mathbf{q} \rightarrow 0) = \frac{\tilde{q} r_s}{2\sqrt{2}} \left( -\frac{\partial^2 \epsilon^{xc}}{\partial \zeta^2} + \text{sign}(\sigma) \frac{r_s}{2} \frac{\partial^2 \epsilon^{xc}}{\partial r_s \partial \zeta} \right), \quad (4)$$

where  $\tilde{q} = \mathbf{q}/k_F$  is the normalized momentum,  $\epsilon^{xc} = E^{xc}/N$  is the exchange and correlation energy per parti-

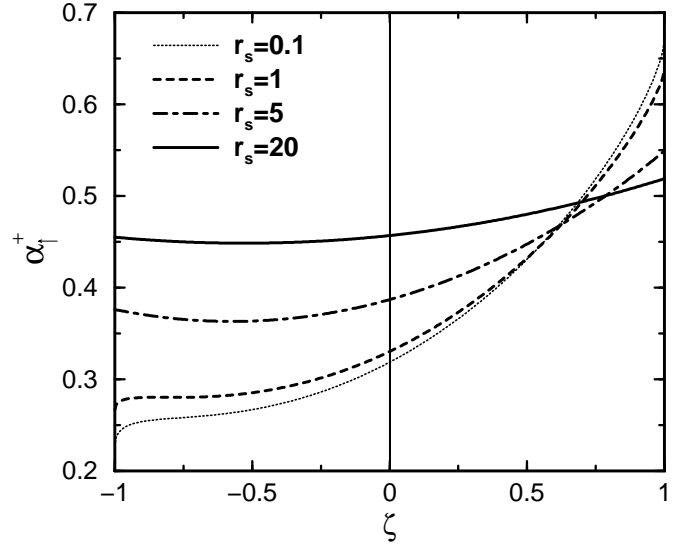


FIG. 1: Initial slope  $\alpha_+^+(r_s, \zeta)$  of the local field factor as a function of the polarization,  $\zeta$ , for  $r_s = 0.1$  (dotted line),  $r_s = 1$  (dashed line),  $r_s = 5$  (dot-dashed line) and  $r_s = 20$  (solid line).

cle measured in Rydbergs and the coupling strength,  $r_s$ , is measured in units of the effective Bohr radius of the system.<sup>13</sup> Using the explicit expression of the exchange energy the local field functions become:

$$G_\uparrow^+(\mathbf{q} \rightarrow 0) = \frac{\tilde{q}}{2\pi} \left( (2 + \zeta) \sqrt{1 + \zeta} - \zeta \sqrt{1 - \zeta} \right) + \frac{\tilde{q} r_s^2}{8\sqrt{2}} \left( \frac{\partial \epsilon^c}{\partial r_s} - r_s \frac{\partial^2 \epsilon^c}{\partial r_s^2} + 2 \frac{\partial^2 \epsilon^c}{\partial r_s \partial \zeta} \right), \quad (5)$$

$$G_\uparrow^-(\mathbf{q} \rightarrow 0) = \frac{\tilde{q}}{2\pi} \left( \frac{2 + \zeta}{\sqrt{1 + \zeta}} + \frac{\zeta}{\sqrt{1 - \zeta}} \right) + \frac{\tilde{q} r_s}{2\sqrt{2}} \left( -\frac{\partial^2 \epsilon^c}{\partial \zeta^2} + \frac{r_s}{2} \frac{\partial^2 \epsilon^c}{\partial r_s \partial \zeta} \right). \quad (6)$$

Similar expressions apply to  $G_\downarrow^\pm$  due to the fact that  $G_\downarrow^\pm(\zeta) = G_\uparrow^\pm(-\zeta)$ .

The inclusion of the correlation energy in the small  $\mathbf{q}$  limit of the local field factors is crucial to correctly evaluate the response functions. If only the exchange contribution to the local field factors is included, the magnetic susceptibility of the unpolarized gas develops a pole for  $r_s \geq \pi/\sqrt{2} \sim 2.221$ ,<sup>17</sup> in disagreement with the results of extensive numerical calculations that show a stable paramagnetic phase up to  $r_s \lesssim 26$ .<sup>18,19</sup> The addition of the correlation energy in the the small  $\mathbf{q}$  limit of the local field factors prevents the occurrence of an instability in the unpolarized electron gas.

To precisely evaluate the contribution from the correlation energy to  $G_\sigma^\pm(\mathbf{q} \rightarrow 0)$  we use the latest numerical computation of the ground-state energy of the two-dimensional electron gas. Following Attaccalite et al.,<sup>19</sup>

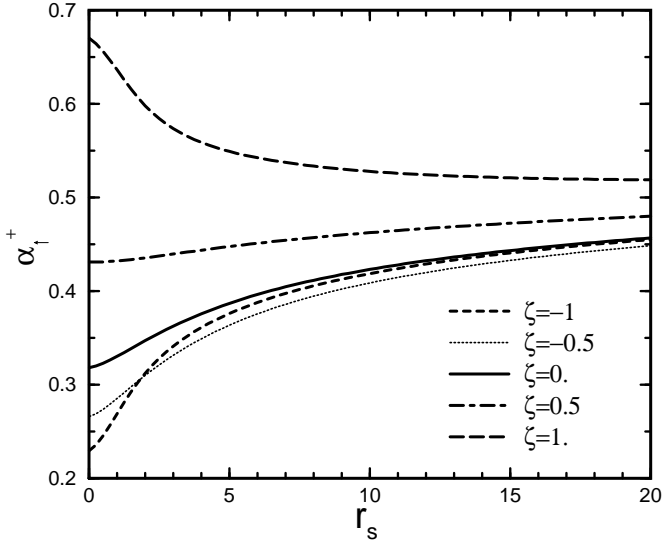


FIG. 2: Initial slope  $\alpha_{\uparrow}^{+}(r_s, \zeta)$  of the local field correction as a function of the coupling strength  $r_s$  for different values of the spin polarization:  $\zeta = -1$  (dashed line),  $\zeta = -0.5$  (dotted line),  $\zeta = 0$  (solid line),  $\zeta = 0.5$  (dot-dashed line) and  $\zeta = 1$  (long-dashed line).

the correlation energy per particle is given by:

$$\epsilon_c(r_s, \zeta) = (e^{-\beta r_s} - 1)\epsilon_x^{(6)}(r_s, \zeta) + \alpha_0(r_s) + \alpha_1(r_s)\zeta^2 + \alpha_2(r_s)\zeta^4, \quad (7)$$

where  $\epsilon_x^{(6)}$  is the Taylor expansion of the exchange energy beyond fourth order in  $\zeta$ ,  $\beta$  is a parameter and the functions  $\alpha_i(r_s)$  are a generalization of previous expressions.<sup>20</sup> By taking the appropriate derivatives of Eq. (7), we derive analytical expressions for the initial slope of the static local field correction functions:  $\alpha_{\sigma}^{\pm} = G_{\sigma}^{\pm}(\tilde{q} \rightarrow 0)/\tilde{q}$ .

The behavior of  $\alpha_{\uparrow}^{+}(r_s, \zeta)$  and  $\alpha_{\uparrow}^{-}(r_s, \zeta)$  is quite different.<sup>21</sup> Fig. 1 shows  $\alpha_{\uparrow}^{+}(r_s, \zeta)$  as a function of the polarization for several values of  $r_s$ . Note that  $\alpha_{\uparrow}^{+}$  is always positive, as the local effects always decrease the uniform electron density at large inter-electronic distances. Also note that  $\alpha_{\uparrow}^{+}$  for small values of  $r_s$  is a monotonically increasing function of  $\zeta$ . This behavior can be understood analyzing the contribution from the exchange interaction given by  $\alpha_x^{+} = [(2 + \zeta)\sqrt{1 + \zeta} - \zeta\sqrt{1 - \zeta}]/2\pi$ . Since the exchange interaction takes place only between electrons with parallel spin, increasing values of  $\zeta$  induce larger effects and further reduction of the uniform electron density at small  $\mathbf{q}$ . Consequently, the value of  $\alpha_{\uparrow}^{+}$  increases. The exchange contribution  $\alpha_x^{+}$ , which does not depend on  $r_s$ , dominates at large electronic densities. However, correlation effects become more important with increasing  $r_s$  and they partly cancel the strong  $\zeta$  dependence of  $\alpha_x^{+}$ , as it can be seen on Fig. 1.

Fig. 2 displays  $\alpha_{\uparrow}^{+}(r_s, \zeta)$  as a function of  $r_s$  for different values of the spin polarization. It can be noticed that

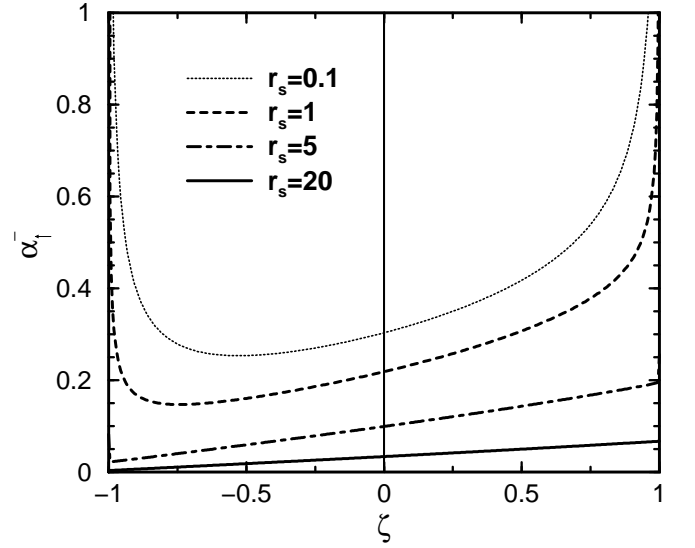


FIG. 3: Initial slope  $\alpha_{\uparrow}^{-}(r_s, \zeta)$  of the local field factor as a function of the polarization for different values of  $r_s$  as indicated in the legend.

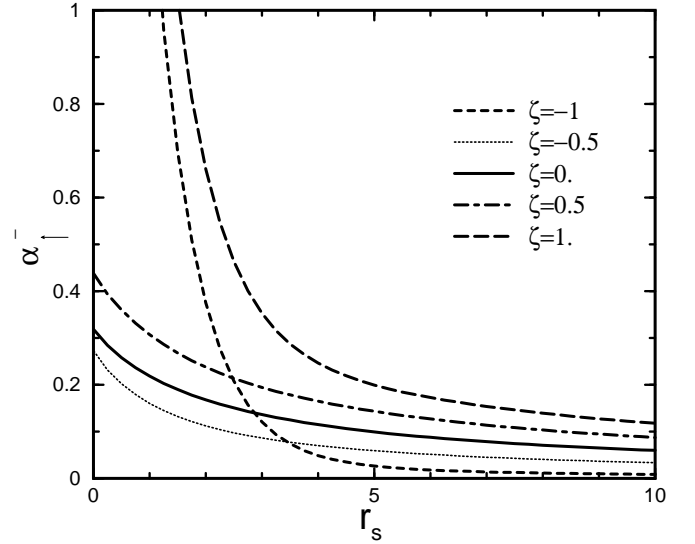


FIG. 4: Initial slope  $\alpha_{\uparrow}^{-}(r_s, \zeta)$  as a function of  $r_s$  for different values of the spin polarization.

$\alpha_{\uparrow}^{+}$  is a monotonic increasing function of  $r_s$  for values of  $\zeta \lesssim 0.5$ . This feature is also displayed on Fig. 1. In particular, as previously noticed,<sup>12</sup> in the unpolarized electron gas  $\alpha_{\uparrow}^{+}(r_s, \zeta = 0)$  increases with  $r_s$ .

Fig. 3 displays the initial slope  $\alpha_{\uparrow}^{-}(r_s, \zeta)$  as a function of  $\zeta$  for different values of  $r_s$ . As in the case of  $\alpha_{\uparrow}^{+}$ , the main contribution for small values of  $r_s$  came from the exchange energy:  $\alpha_x^{-} = \frac{1}{2\pi} \left( \frac{2 + \zeta}{\sqrt{1 + \zeta}} + \frac{\zeta}{\sqrt{1 - \zeta}} \right)$ . Therefore, for large electronic densities  $\alpha_{\uparrow}^{-}$  diverges for a fully polarized system ( $\zeta = \pm 1$ ), behavior explained by the

fact that in a fully polarized gas the magnetic susceptibility becomes zero. As  $r_s$  increases, correlation effects quench by a factor of  $e^{-\beta r_s}$  the diverging contribution from the exchange energy.<sup>22</sup> Thus, correlation effects become dominant at small densities and the strong dependence of  $\alpha_x^-$  with  $\zeta$  is completely washed out. Instead, at large values of  $r_s$ ,  $\alpha_x^-$  becomes a linear function of  $\zeta$ .

Fig. 4 displays  $\alpha_{\uparrow}^-(r_s, \zeta)$  as a function of  $r_s$  for different values of the spin polarization. The divergence at  $r_s = 0$  and  $\zeta = \pm 1$  is clearly displayed. Note that  $\alpha_{\uparrow}^-$  is a monotonic decreasing function of  $r_s$  for any value of  $\zeta$ .

### B. Large wavevector

In the limit of large wavevector it is easier to derive independently expressions for  $\tilde{G}_{\sigma}^{\pm}$  and for  $G_{\sigma}^n$ . For large frequency or large wavevector, an iterative method generates the exact asymptotic expressions for  $\tilde{G}_{\sigma}^{\pm}$ .<sup>23</sup> For a two-dimensional electron gas,<sup>11</sup>

$$\tilde{G}_{\uparrow}^+(\mathbf{q} \rightarrow \infty) = \beta_{\uparrow}^+(r_s, \zeta) = 1 - \frac{1}{2}g_{\uparrow\downarrow}(0) \quad (8)$$

$$\tilde{G}_{\uparrow}^-(\mathbf{q} \rightarrow \infty) = \beta_{\uparrow}^-(r_s, \zeta) = \frac{1}{2}g_{\uparrow\downarrow}(0) \quad (9)$$

where  $g_{\uparrow\downarrow}(0)$  is the spin resolved pair distribution function at the origin. It has been shown that  $g_{\uparrow\downarrow}(0)$  is largely unaffected by the degree of spin polarization.<sup>24,25</sup> In our calculation we use the simple expression  $g_{\uparrow\downarrow}(0) = \frac{1}{[1 + 0.6032 r_s + 0.07263 r_s^2]^2}$ , where only the parameter  $r_s$  appears.<sup>25</sup> With this choice,  $\beta_{\uparrow}^+(r_s, \zeta) = \beta_{\downarrow}^+(r_s, \zeta) = \beta^+(r_s)$  and  $\beta_{\uparrow}^-(r_s, \zeta) = \beta_{\downarrow}^-(r_s, \zeta) = \beta^-(r_s)$ .

In order to calculate the large momentum behavior of  $G_{\sigma}^n$  we need to approximate the modified polarization function,<sup>9,26</sup>

$$\Pi_{\sigma\sigma'}(\mathbf{q}, \omega) = \frac{1}{A} \sum_{\mathbf{k}} \frac{\bar{n}_{\mathbf{k},\sigma} - \bar{n}_{\mathbf{k}+\mathbf{q},\sigma'}}{\omega + \xi_{\mathbf{k}\sigma} - \xi_{\mathbf{k}+\mathbf{q}\sigma'}} \quad (10)$$

where  $\xi_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + \text{sign}(\sigma)\gamma^*B = k^2/2m + \text{sign}(\sigma)\gamma^*B$  is the quasiparticle energy in the static magnetic field  $B$ ,  $\bar{n}_{\mathbf{k},\sigma}$  is the exact occupation numbers in the interacting electron gas, and  $A$  is the area of the system. Since at large  $\mathbf{q}$  the particle number renormalization is the dominant effect, Eq. (10) neglects the renormalization of the quasiparticle effective mass.

By making an asymptotic expansion of the interacting polarization function,<sup>26</sup> the local factor  $G_{\sigma}^n$  can be written down as,<sup>27,28</sup>

$$G_{\sigma}^n(\mathbf{q} \rightarrow \infty) = \frac{r_s}{\sqrt{2}} \frac{\Delta t_{\sigma}}{(1 + \zeta)^2} \tilde{q} = \gamma_{\sigma}(r_s, \zeta) \tilde{q} \quad (11)$$

where  $\tilde{q} = \mathbf{q}/k_F$  is the normalized momentum,  $\tilde{k}_{F\sigma} = k_{F\sigma}/k_F$  the normalized Fermi momentum of the spin  $\sigma$  electronic population and  $\Delta t_{\sigma} = t_{\sigma} - t_{\sigma}^0$  is the difference

between the kinetic energy of the electrons with spin  $\sigma$  in the interacting system,  $t_{\sigma} = \frac{1}{N} \sum_{\mathbf{k}} \bar{n}_{\mathbf{k}\sigma} \frac{k^2}{2m}$ , and in the non-interacting gas,  $t_{\sigma}^0 = \frac{1}{N} \sum_{\mathbf{k}} n_{\mathbf{k}\sigma}^0 \frac{k^2}{2m}$ , over the total number of electrons. This equation is valid when  $\Delta t_{\sigma}$  is measured in Rydbergs and  $r_s$  in units of the effective Bohr radius.<sup>13</sup>

The difference in kinetic energies can be related with the exchange and correlation energies and their derivatives using the virial<sup>29</sup> and the magnetic virial theorems:<sup>11</sup>

$$\Delta t_{\sigma} = -\frac{r_s}{2} \frac{\partial(\epsilon^x + \epsilon^c)}{\partial r_s} - \epsilon_{\sigma}^x - \epsilon_{\sigma}^c \quad (12)$$

where  $\epsilon^x = E^x/N$  and  $\epsilon^c = E^c/N$  are, respectively, the average exchange and correlation energy per particle;  $\epsilon_{\sigma}^x = E_{\sigma}^x/N$  and  $\epsilon_{\sigma}^c = E_{\sigma}^c/N$  are the average exchange and correlation energy of the electrons with spin  $\sigma$ .

The average exchange energy for any spin population is well known:  $\epsilon_{\sigma}^x = -\frac{4\sqrt{2}}{3\pi r_s} (1 + \text{sign}(\sigma)\zeta)^{3/2}$  (Ry). The spin dependent correlation energies are difficult to evaluate or to extract from numerical calculations. Therefore, we have to rely on same approximate scheme to extract the spin dependent correlation energy from the available computations of the full correlation energy. The total correlation energy per particle is  $\frac{E^c}{N} = \epsilon_{\uparrow}^c + \epsilon_{\downarrow}^c = \tilde{\epsilon}_{\uparrow}^c \frac{1+\zeta}{2} + \tilde{\epsilon}_{\downarrow}^c \frac{1-\zeta}{2}$ . Perdew and Wang<sup>20</sup> suggested the following parameterization for the correlation energy of a polarized electron gas:

$$\epsilon^c(r_s, \zeta) = \epsilon^c(r_s, 0) + h(r_s, \zeta)f(\zeta) \quad (13)$$

where  $h(r_s, \zeta)$  is an even function of the polarization and  $f(\zeta) = \frac{(1+\zeta)^{3/2} + (1-\zeta)^{3/2} - 2}{2(\sqrt{2} - 1)}$  for a two-dimensional system.<sup>12</sup> This function can be decomposed as  $f(\zeta) = [f_{\uparrow}(\zeta)(1+\zeta) + f_{\downarrow}(\zeta)(1-\zeta)]/2$ , where  $f_{\sigma} = [\sqrt{1 + \text{sign}(\sigma)\zeta} - 1]/[\sqrt{2} - 1]$ . An estimate of the spin dependent correlation energies can be obtained as:

$$\epsilon_{\sigma}^c(r_s, \zeta) = \frac{1 + \text{sign}(\sigma)\zeta}{2} \tilde{\epsilon}_{\sigma}^c(r_s, \zeta), \quad \text{where} \quad \tilde{\epsilon}_{\sigma}^c(r_s, \zeta) = \epsilon^c(r_s, 0) + \frac{f_{\sigma}(\zeta)}{f(\zeta)} [\epsilon^c(r_s, \zeta) - \epsilon^c(r_s, 0)]. \quad (14)$$

Using the parameterization of the correlation energy proposed in Ref. 19, Eq. (7), we obtain reasonable values for  $\epsilon_{\sigma}^c$ . Also, its dependence with the polarization is the expected one. At a fixed value of  $r_s$ ,  $\epsilon_{\uparrow}^c$  ( $\epsilon_{\downarrow}^c$ ) is a monotonic increasing (decreasing) function of  $\zeta$ .

Fig. 5 shows the dependence of  $\gamma_{\uparrow}(r_s, \zeta)$ , Eq. (11), with the polarization for several values of  $r_s$ . While the initial slopes ( $\alpha_{\sigma}^{\pm}$ ) and the constant terms in the large  $\mathbf{q}$  limit

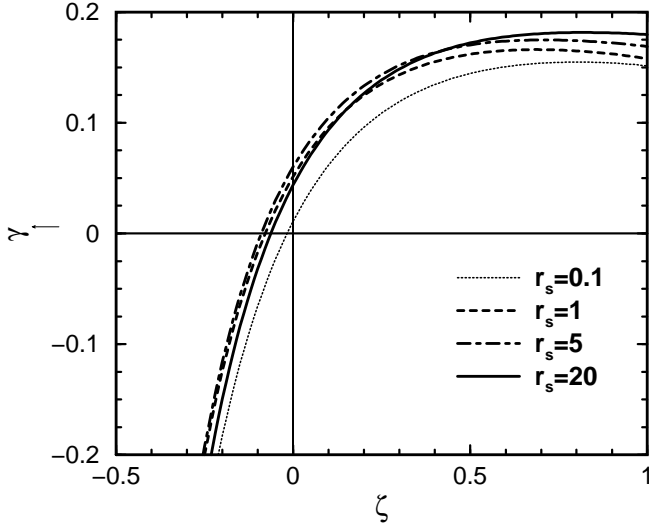


FIG. 5: The coefficient  $\gamma_{\uparrow}(r_s, \zeta)$  as a function of  $\zeta$  for different values of  $r_s$  as indicated in the legend.

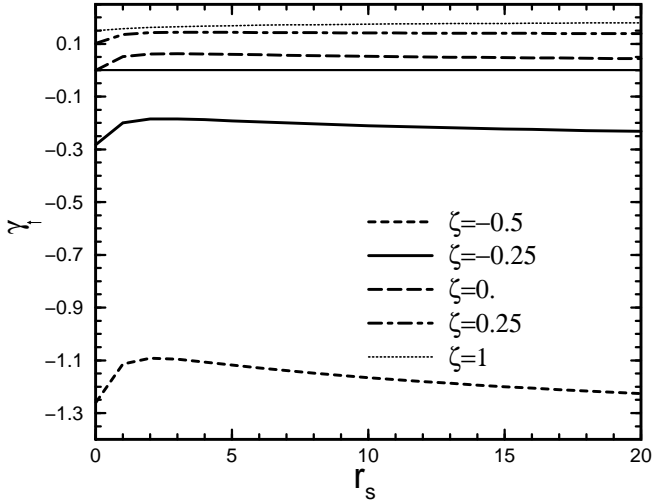


FIG. 6: The coefficient  $\gamma_{\uparrow}(r_s, \zeta)$  as a function of the coupling strength  $r_s$  for different values of the polarization:  $\zeta = -0.5$  (dashed line),  $\zeta = -0.25$  (solid line),  $\zeta = 0$  (long-dashed line),  $\zeta = 0.25$  (dot-dashed line) and  $\zeta = 1$  (dotted line).

( $\beta^{\pm}$ ) of the local factors are always positive, the coefficient  $\gamma_{\sigma}$  can have any sign. Since  $\gamma_{\sigma} \propto \Delta t_{\sigma}$ , a change in sign of  $\gamma_{\sigma}$  implies a change of sign of  $\Delta t_{\sigma} = t_{\sigma} - t_{\sigma}^0$ . Even though, for a given spin  $\Delta t_{\sigma}$  can be negative, the difference in the total kinetic energies of the interacting and the non-interacting system,  $\Delta T = N[\Delta t_{\uparrow} + \Delta t_{\downarrow}]$ , is positive for any value of  $\zeta$  and  $r_s$ .<sup>26</sup>

The negative value of  $\Delta t_{\uparrow}$  for negative polarizations is easily understood if the variation with the polarization of the carrier effective mass is considered. It is well known that in a polarized electron gas the mass of the minority (majority) spin populations increases (decreases) with the value of the polarization.<sup>30</sup> Therefore, for large

enough values of  $\zeta$  the mass renormalization dominates, and the kinetic energy of the minority (majority) carriers is reduced (increased) with respect to its free electron value. Also, as  $\zeta$  increases, the exchange effects between the minority (majority) spins are greatly reduced (increased). Due to the combination of these two effects the electrons from the majority spin population will tend to accumulate around the few minority spins increasing the local charge around them. This generates a negative value of  $G^n(\mathbf{q} \rightarrow \infty)$  for the minority spins. The opposite is true for the majority spins.

At finite values of the polarization, the kinetic energy of each spin population is dominated by the exchange contribution,  $\Delta t_{\sigma} = -\frac{r_s}{2} \frac{\partial \epsilon^x}{\partial r_s} - \epsilon_{\sigma}^x \sim \zeta/r_s$ , a behavior that is independent of the parameterization used to obtain the spin-dependent correlation energy, Eq. (14) in our case. At large values of  $r_s$ , the correlation effects become more important as it can be seen on Fig. 5. Finally, we point out that the large effect of the polarization in the value of  $\gamma_{\uparrow}(r_s, \zeta)$  is mainly due to the denominator  $(1 + \zeta)^2$  of Eq. (11).

Fig. 6 displays  $\gamma_{\uparrow}(r_s, \zeta)$  as a function of  $r_s$  for several values of  $\zeta$  between  $\zeta = -0.5$  and  $\zeta = 1$ . The same trends as in Fig. 5 become apparent: strong dependence on  $\zeta$  and weak dependence with  $r_s$ . For values of  $\zeta < 1$ ,  $\gamma_{\uparrow}$  increases with  $r_s$ , reaches a maximum and decreases afterwards. For example, for  $\zeta = 0$  the maximum is reached at  $r_s = 2.88$ . For  $\zeta = 1$ ,  $\gamma_{\uparrow}$  monotonically increases with  $r_s$ .

### III. SPIN DEPENDENT LOCAL FIELD CORRECTIONS

Numerous parametrized expressions of the local field factors for the unpolarized three-<sup>6,31,32,33</sup> and two-dimensional<sup>27,34,35</sup> electron gas has been suggested since the pioneering work of Hubbard.<sup>36</sup> All these parametrized schemes rely on finding a function of the electronic density that smoothly interpolates between the short and long wavelength limits of the local field factors. However, parametrized expressions of  $G^{\pm}$  for the polarized gas have not received so much attention. Numerical calculations in the polarized electron gas are also computationally challenging and, so far, only results for the ground state energy and the pair-distribution functions are available.<sup>18,19,37,38</sup>

As we have discussed in the previous section, at small values of  $\mathbf{q}$  the local factors follow a linear dependence,  $G_{\sigma}^{\pm}(\mathbf{q} \rightarrow 0) = \alpha_{\sigma}^{\pm}(r_s, \zeta) \tilde{q}$ , where  $\tilde{q} = \mathbf{q}/k_F$ . In the opposite end of the spectrum the local corrections follow a linear plus constant dependence,  $G_{\sigma}^{\pm}(\mathbf{q} \rightarrow \infty) = \beta^{\pm}(r_s) + \gamma_{\sigma}(r_s, \zeta) \tilde{q}$ . Given the diversity of behaviors displayed by the parameters  $\alpha_{\sigma}^{\pm}$ ,  $\beta^{\pm}$  and  $\gamma_{\sigma}$ , we will consider a general interpolating scheme for all values of  $r_s$  and  $\zeta$ . We parametrized  $G^{\pm}$  with two fitting parameters,

TABLE I: Optimal fit parameters for the local field factors as parametrized in Eqs. (15) and (16).

	i=0	i=1		i=0	i=1
$a_i^+$	2.4847	2.6523	$a_i^-$	3.0578	3.9225
$b_i^+$	0.6972	0.1927	$b_i^-$	0.6844	0.6407
$c_i^+$	0.4371	0.1384	$c_i^-$	1.2545	0.2507

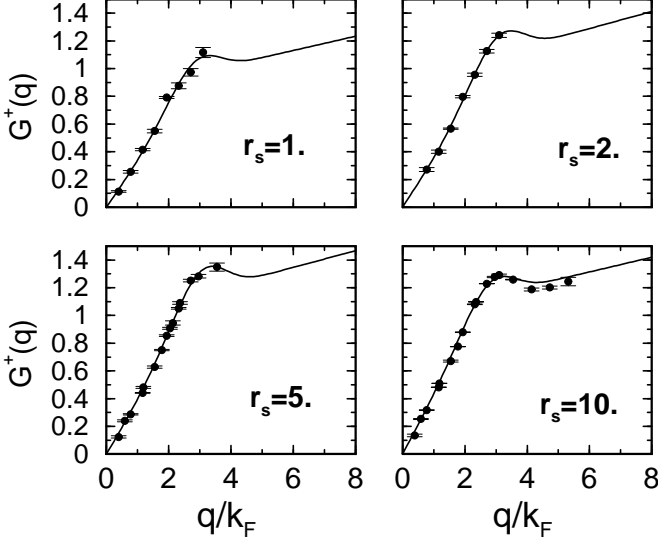


FIG. 7: Local field correction factor  $G^+(\mathbf{q}, \omega = 0)$  versus normalized momentum  $\mathbf{q}/k_F$  for  $r_s = 1, 2, 5$  and  $10$ . Black circles correspond to the diffusion Monte Carlo (DMC) results of Ref. 12 and solid lines are calculated according to Eqs. (15) and (16).

$q_0^\pm$  and  $q_1^\pm$  as:

$$G_\sigma^\pm(\mathbf{q}) = \alpha_\sigma^\pm \tilde{q} e^{-(\tilde{q}/q_0^\pm)^4} + (\beta^\pm + \gamma_\sigma \tilde{q}) [1 - e^{-(\tilde{q}/q_1^\pm)^4}]. \quad (15)$$

The fast decreasing exponential factors  $\exp[-(\tilde{q}/q_0^\pm)^4]$  and  $\exp[-(\tilde{q}/q_1^\pm)^4]$  are needed to mimic the rapid evolution of the local functions from their small  $\mathbf{q}$  to their large  $\mathbf{q}$  limiting behaviors. This fast evolution is clearly displayed on the latest diffusion Monte Carlo (DMC) results,<sup>12</sup> which show how the local factors  $G^+(\mathbf{q})$  and  $G^-(\mathbf{q})$  of the unpolarized gas follow the predicted linear dependence at small values of the wavevector and rapidly reach their asymptotic large wavevector limits at not very large values of  $\tilde{q}$ . Since there are only numerical results for the unpolarized electron gas, we consider the parameters  $q_0^\pm$  and  $q_1^\pm$  as functions only on the electron density. By fitting Eq. (15) to the DMC results of Ref. 12 we find that the two fitting parameters are smoothly varying functions of the coupling strength and can be parametrized as:

$$q_i^\pm = \frac{a_i^\pm + b_i^\pm r_s + c_i^\pm r_s^{3/2}}{1 + \frac{1}{2} c_i^\pm r_s^{3/2}}, \quad (16)$$

where the parameters  $a_i^\pm$ ,  $b_i^\pm$  and  $c_i^\pm$  are given in Table I.

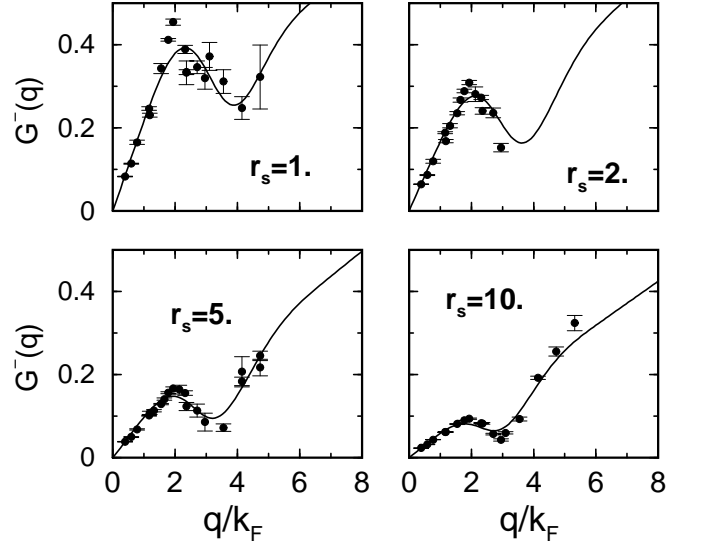


FIG. 8: Local field correction factor  $G^-(\mathbf{q}, \omega = 0)$  versus normalized momentum  $\mathbf{q}/k_F$  for the same values of  $r_s$ . Black circles correspond to the diffusion Monte Carlo (DMC) results of Ref. 12 and solid lines are calculated according to Eqs. (15) and (16).

In Fig. 7 we compared our results for  $G^+(\mathbf{q})$  of the unpolarized electron gas at  $r_s = 1, 2, 5$  and  $10$ , Eqs. (15) and (16), with the DMC results.<sup>12</sup> In Fig. 8 our results for  $G^-(\mathbf{q})$  of the unpolarized electron gas are also compared with the numerical equivalent data. It is clear that our parametrized expressions agree very well with the Quantum Monte Carlo results.<sup>12</sup> By adding more free parameters to Eq. (15) the agreement with the numerical results will improve, but the question of how the parameters of the fit evolve with the spin polarization remains, as yet, unanswered. Thus, we keep the parameterization as simple as possible: our fitting scheme, Eq. (15), is the same for both local functions, it contains only two free parameters and these two parameters have the same functional dependence with the electronic density, Eq. (16).

Fig. 9 shows the momentum dependence of the local field functions  $G_\sigma^+(\mathbf{q})$  for three values of the polarization,  $\zeta = 0, 0.5$  and  $0.9$ , and two values of the coupling strength,  $r_s = 2$  (density of  $7.43 \cdot 10^{10} \text{ cm}^{-2}$  in GaAs) and  $r_s = 10$  (density of  $0.297 \cdot 10^{10} \text{ cm}^{-2}$  in GaAs). The factor associated with the majority spins,  $G_\uparrow^+$ , behaves quite different from the one of the minority spins,  $G_\downarrow^+$ . The field factor  $G_\uparrow^+$  is always positive for positive values of the polarization. It slightly increases with the degree of polarization, but it keeps the characteristic peak of the unpolarized local factor around the same value of  $\mathbf{q}$ . This peak is a residue of the sharp peak in the exchange potential,<sup>39</sup> which is washed out and/or shifted to higher values of  $\mathbf{q}$  by the inclusion of short-range correlations.<sup>16</sup> On the other hand, the behavior of  $G_\downarrow^+$  is dominated by the forced change in its slope, from a positive value at small  $\mathbf{q}$  to a large negative value at large wavevectors. As

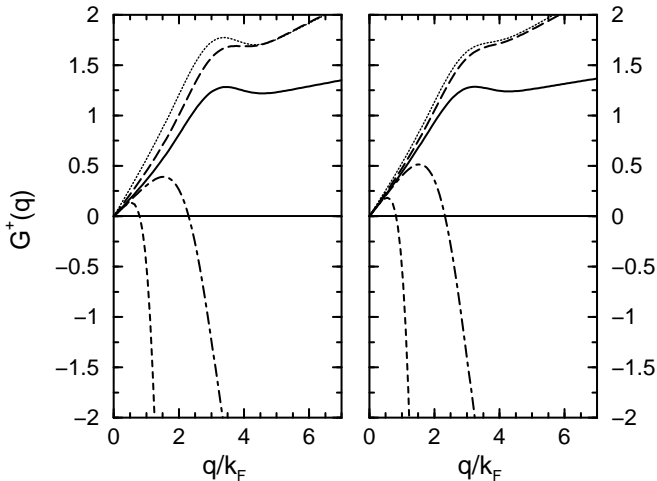


FIG. 9: Local field corrections  $G^+_{\sigma}(\mathbf{q}, \omega = 0)$  versus normalized momentum  $\mathbf{q}/k_F$  for a two dimensional electron gas with  $r_s = 2$  (left panel) and  $r_s = 10$  (right panel). Results for  $G^+$  at  $\zeta = 0$  (solid lines),  $G^+_{\uparrow}$  (long-dashed lines) and  $G^+_{\downarrow}$  (dot-dashed lines) at  $\zeta = 0.5$ , and  $G^+_{\uparrow}$  (dotted lines) and  $G^+_{\downarrow}$  (dashed lines) at  $\zeta = 0.9$  are displayed.

a result,  $G^+_{\downarrow}$  has always a maximum, whose position shifts to lower values of  $\tilde{q}$  with increasing  $\zeta$  and it is strongly dependent on the precise parameterization used. For example, it can shift to larger values of  $\tilde{q}$  if  $q_0^+$  and  $q_1^+$  are also functions of  $\zeta$ . This issue should be explored in greater detail. Finally, by comparing the field factors for  $r_s = 2$  and  $r_s = 10$  we conclude that their dependence on  $r_s$  is weak.

Fig. 10 displays the local field factor  $G^-_{\sigma}(\mathbf{q})$  versus normalized momentum for the same values of  $\zeta$  and  $r_s$  used in Fig. 9. The main difference between  $G^+_{\uparrow}(\mathbf{q})$  and  $G^-_{\uparrow}(\mathbf{q})$  is that the latest one displayed a sharper peak around  $\tilde{q} \sim 2$ . It appears that higher order effects, which are important in the computation of  $G^+_{\uparrow}$ , cancel out in calculations of  $G^-_{\uparrow}$  due to the antisymmetric averaging over spin.<sup>14</sup> It is also noticeable how the local factors change with increasing  $r_s$ .

#### IV. CONCLUSIONS

We have considered an analytic parameterization of the spin dependent local field factors of the polarized two-dimensional electron gas, Eqs. (15) and (16). Our parameterization incorporates the known asymptotic limits of the local corrections and gives an accurate fit of the available quantum Monte Carlo data.<sup>12</sup> We found that the local field corrections associated to the minority spins strongly depend on the polarization, while the local field functions of the majority spins are less affected by the

degree of polarization. This is mainly due to the negative value of the linear term on the large  $\mathbf{q}$  limit of the

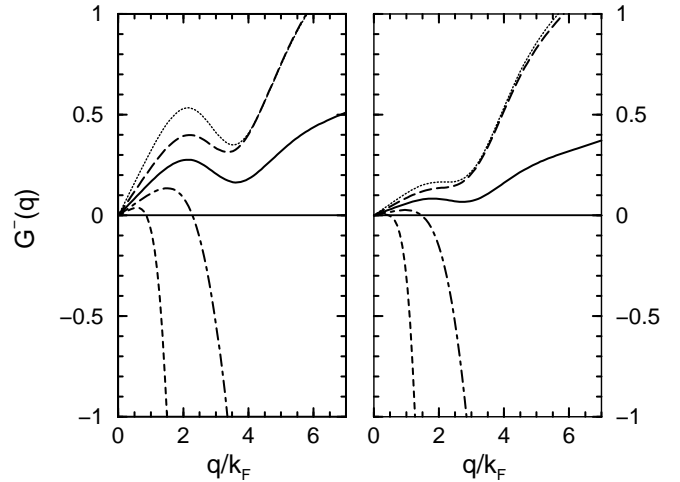


FIG. 10: Local field corrections  $G^-_{\sigma}(\mathbf{q}, \omega = 0)$  versus normalized momentum  $\mathbf{q}/k_F$  for a two dimensional electron gas with  $r_s = 2$  (left panel) and  $r_s = 10$  (right panel). Results for  $G^-$  at  $\zeta = 0$  (solid lines),  $G^-_{\uparrow}$  (long-dashed lines) and  $G^-_{\downarrow}$  (dot-dashed lines) at  $\zeta = 0.5$ , and  $G^-_{\uparrow}$  (dotted lines) and  $G^-_{\downarrow}$  (dashed lines) at  $\zeta = 0.9$  are included.

local field factors of the minority spins.

The analytic parameterization used has only two parameters which have been fitted to reproduce the latest DMC results for the unpolarized electron gas.<sup>12</sup> Since, that there are not data on polarized systems we have considered these two parameters as functions only on the electron density. Therefore, further study will be needed to evaluate their dependence on the spin polarization and the efficacy of our parameterization at large values of  $\zeta$ .

In conclusion, we believe that our approach provides a realistic qualitative description of the paramagnetic phase of the polarized electron gas. Caution, however, should be exercised in applying our calculation in the limit of  $\zeta$  approaching unity, where the paramagnetic model breaks down. We have found that for small values of  $r_s$  and large values of  $\zeta$ , the magnetic susceptibility and the inverse dielectric constant develop a pole at the same value of the electronic density and the spin polarization. This fact signals a charge-spin density wave instability in the polarized electron gas and it will be discussed elsewhere.<sup>40</sup>

#### Acknowledgments

We are grateful to Dr. Moroni and Dr. Senatore for providing us with the results of their numerical calculation of the local field factors in the unpolarized electron gas. We gratefully acknowledge the financial support provided by the Department of Energy, grant no. DE-FG02-01ER45897.

- <sup>1</sup> S. A. Crooker, D. A. Tulchinsky, J. Levy, D. D. Awschalom, R. Garcia and N. Samarth, Phys. Rev. Lett. **75**, 505 (1995).
- <sup>2</sup> For a review, see G. Prinz and K. Hathaway, Physics Today, **48**, (4), 24.
- <sup>3</sup> G. D. Mahan in *Many-Particle Physics*, chapter 5 (Plenum Press, New York, 1990).
- <sup>4</sup> K. S. Yi and J. J. Quinn, Phys. Rev. B **54**, 13398 (1996).
- <sup>5</sup> C. A. Kukkonen and A.W. Overhauser, Phys. Rev. B **20**, 550 (1979).
- <sup>6</sup> X. Zhu and A. W. Overhauser, Phys. Rev. B **33**, 925 (1986).
- <sup>7</sup> In an unpolarized electron gas,  $G^+$  appears only in the expressions of the electrical response functions, and  $G^-$  only on the magnetic response susceptibilities. However, in a polarized electron system the four local field factors appear in all the response functions.
- <sup>8</sup> D. C. Marinescu and J. J. Quinn, Phys. Rev. B **56**, 1114 (1997).
- <sup>9</sup> C. F. Richardson and N. W. Ashcroft, Phys. Rev. B, **50**, 8170 (1994); **55**, 15130 (1997).
- <sup>10</sup> D. C. Marinescu and I. Tifrea, Phys. Rev. B **65**, 113201 (2002).
- <sup>11</sup> M. Polini and M. P. Tosi, Phys. Rev. B **63**, 045118 (2001).
- <sup>12</sup> S. Moroni, D. M. Ceperley and G. Senatore, Phys. Rev. Lett. **69**, 1837 (1992); Phys. Rev. Lett. **75**, 689 (1995); G. Senatore, S. Moroni and D. M. Ceperley, in *Quantum Monte Carlo Methods in Physics and Chemistry*, edited by M. P. Nightingale and C. J. Umrigar (Kluwer, 1999); G. Senatore, S. Moroni and D. Varsano, Solid State Commun. **119**, 333 (2001); private communication.
- <sup>13</sup> Where  $a_B^*$  is the effective Bohr radius of the system,  $a_B^* = \hbar^2/(m^*e^2)$ . For a regular three dimensional metal  $a_B^* = a_0 = 0.529 \cdot 10^{-8}$  cm and  $a_B^* = 195 a_0 = 1.04 \cdot 10^{-6}$  cm for GaAs.
- <sup>14</sup> G. S. Atwal and N. W. Ashcroft, to be published.
- <sup>15</sup> A. Holas, P. K. Aravind and K. S. Singwi, Phys. Rev B **20**, 4912 (1979); P. K. Aravind, A. Holas, and K. S. Singwi, Phys. Rev. B **25**, 561 (1982).
- <sup>16</sup> F. Pederiva, E. Lipparini and K. Takayanagi, Europhysics Lett., **40**, 607 (1997).
- <sup>17</sup> The dielectric function also develops a pole at the same value of the coupling strength. However, a pole in the dielectric function indicates not an instability of the paramagnetic phase but a region in momentum space where the Coulomb interaction is overscreened. See O. V. Dolgov, D. A. Kirzhnits and E. G. Maksimov, Rev. of Mod. Phys. **53**, 81 (1981) and references therein.
- <sup>18</sup> B. Tanatar and D. M. Ceperley, Phys. Rev. Phys. B **39**, 5005 (1989).
- <sup>19</sup> C. Attaccalite, S. Moroni, P. Gori-Giorgi and G. B. Bachelet, Phys. Rev. Lett. **88**, 256601 (2002).
- <sup>20</sup> J. P. Perdew and Y. Wang, Phys. Rev. B, **45**, 13244 (1992).
- <sup>21</sup> Similar arguments apply to  $\alpha_{\uparrow}^{\pm}(r_s, \zeta)$ .
- <sup>22</sup> The quenching of the divergence at  $\zeta \pm 1$  will depend on the precise parameterization used for the correlation energy.
- <sup>23</sup> G. Niklasson, Phys. Rev. B **10**, 3052 (1974).
- <sup>24</sup> M. Polini, G. Sica, B. Davoudi and M. P. Tosi, J. Phys.: Condens. Matter **13**, 3591 (2001).
- <sup>25</sup> J. Moreno and D.C. Marinescu, cond-mat/0210137.
- <sup>26</sup> A. Holas, in *Strongly Coupled Plasma Physics*, edited by F.J. Rogers and H.E. DeWitt (Plenum, New York, 1987), p. 463.
- <sup>27</sup> B. Davoudi, M. Polini, G. F. Giuliani and M. P. Tosi, Phys. Rev. B, **64**, 153101 (2001); **64**, 233110 (2001).
- <sup>28</sup> *Quantum Theory of the Electron Liquid* by G. F. Giuliani and G. Vignale (Cambridge University Press), to be published.
- <sup>29</sup> N. H. March, Phys. Rev., **110**, 604 (1958).
- <sup>30</sup> A. W. Overhauser, Phys. Rev. B, **4**, 3318 (1971).
- <sup>31</sup> K. S. Singwi, A. Sjölander, M. P. Tosi and R.H. Land, Phys. Rev B **1**, 1044 (1970).
- <sup>32</sup> P. Vashishta and K. S. Singwi, Phys. Rev B **6**, 875 (1972).
- <sup>33</sup> M. Corradini, R. Del Sole, G. Onida and M. Palumbo, Phys. Rev. B, **57**, 14569 (1998).
- <sup>34</sup> N. Iwamoto, Phys. Rev. B, **43**, 2174 (1991).
- <sup>35</sup> C. Bulutay and M. Tomak, Phys. Rev. B **53**, 7317 (1996).
- <sup>36</sup> J. Hubbard, Proc. R. Soc. London, Ser. A **240**, 539 (1957); **243**, 336 (1957).
- <sup>37</sup> C. Bulutay and B. Tanatar, Phys. Rev. B **65**, 195116 (2002).
- <sup>38</sup> B. Davoudi and M. P. Tosi, cond-mat/0107519.
- <sup>39</sup> Y. R. Wang, M. Ashraf and A. W. Overhauser, Phys. Rev. B, **30**, 5580 (1984).
- <sup>40</sup> J. Moreno and D.C. Marinescu, to be published.